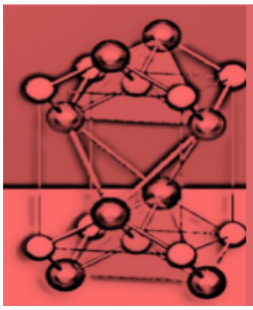

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DFT study of ethanol and formic acid adsorption on CaO(001)

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Ethanol and formic adsorption on CaO (0 0 1) surface at low coverage is studied using Density Functional Theory (DFT) calculations with van der Waals corrections. We investigated the CaO surface in its rock salt structure. The more favorable sites for C_2H_5OH adsorption are on one (or two) Ca cations bonding the O atom from ethanol. H form (OH group) bond to surface oxygens with an adsorption energy of -1.12 (-1.14) eV. The distance of ethanol to surface is in the range of 2.3 - 2.5$\mathring{A}$. The molecule presents a strong elongation of the adsorbed O-H group being 53% (51%) larger that its molecular distance. Bond order analysis shows that distances and BO are similar for Ca-O molecule and Ca-O surface. A charge transfer occurs from O atom of the 2nd layer to Ca ions at 1st layer and the molecular O atom gain some charge, while H loses charge towards surface oxygen and from this to the rest of the surface. In the case of H-COOH we found two possible adsorption sites with -2.38 and -2.07 eV, again the O-H bond is elongated with respect to the molecular states. DOS and bonding analysis are performed in both cases.